Recent advances in computational tools in the fields of protein design and docking is beginning to have significant impact on biotechnology. Development of accurate side-chain placement algorithms and reliable scoring functions are at the heart of these applications.

SCREAM (SideChain Rotamer Energy Analysis Methodology), a side-chain placement program, has been actively used in problems such as the prediction of GPCR's, docking of ligands, and designing of amino-acyl tRNA synthetase (aaRS). With flexibility and accuracy as focus, SCREAM outperforms the standard side-chain placement package SCWRL by about 0.2 Å RMSD per residue for protein side-chain predictions.

Electrostatics has sometimes been referred to as the “bane” of molecular dynamics. Protein have naturally occurring positively and negatively charged groups, and the fluctuations in the positions of these groups leads to large fluctuation in energies, the most commonly used criteria for scoring. Such large variance can be reduced by neutralizing those charged groups by protonation or deprotonation, while sacrificing little. Improvements in correlation of binding data to neutralized energy scoring is observed.